

Benzenesulfonic acid, 2-chloro-5-nitro-, sodium salt
946-30-5 | DTXSID4061339

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 28.2 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.03e-01

Confidence level: 4.85e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Sulfone, methyl pentafluorophenyl</div> <div>Measured: 28.8</div> <div>Predicted: 104</div>	<div>Image not found</div> <div>Dimethipin</div> <div>Measured: 3.02</div> <div>Predicted: 8.86</div>	<div>Image not found</div> <div>Chloranil</div> <div>Measured: 209</div> <div>Predicted: 259</div>
<div>Image not found</div> <div>Picloram</div> <div>Measured: 20.0</div> <div>Predicted: 27.1</div>	<div>Image not found</div> <div>Trichlorfon</div> <div>Measured: 79.4</div> <div>Predicted: 43.7</div>	